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***In situ* X-ray Diffraction Studies of Cathode Materials for Lithium Batteries**

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Beamline(s): X18A, X7A

**Introduction**: Three types of intercalation Compounds, $LiMn_2O_4$ with spinel structure, $LiNiO_2$ and $LiCoO_2$ with layered structure are widely studied as cathode materials for lithium-ion batteries. Among them, $LiCoO_2$ is the most widely used cathode material in commercial lithium battery cells. $LiNiO_2$ has same theoretical capacity as $LiCoO_2$, but is less expensive. However its application in lithium batteries has not been realized due to serious safety concerns. Substituting a portion of Ni in $LiNiO_2$ with other cations has been pursued as a way to improve its safety characteristics. It was reported that Co doped $LiNi_{0.8}Co_{0.2}O_2$ showed better thermal stability than pure $LiNiO_2$. Many new materials have been developed aimed in increasing the capacity and improving the thermal stability and cycleability. Most of these new materials are based on these three types of materials and modified their compositions and structures by doping. However, most of the efforts on developing new cathode materials have been done on the empirical base without guidelines from the systematic studies on the relationship between the performance and the structural changes of the cathode materials. Taking advantage of the strong x-ray beam from the National synchrotron Light Source, we have carried out *in situ* XRD studies on all of these types of cathode materials.

**Results**: Using the state of art synchrotron based *in situ* XRD technique, new phases and new phase transitions during charge have been observed in all of these three systems. These new phases and phase transitions have not been reported or correctly identified in the literature. The relationship between the performance (capacity, thermal stability and cycleability) and the structural changes during cycling has been thoroughly studied. The results are presented in the references listed below.

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